Materials by Computer Design: An Introduction

CAN novel materials with optimized properties be designed by computer? Advances in modeling methods at the atomic level coupled with rapid increases in computer capabilities over the last decade have led scientists to answer this question with a resounding "Yes."

The ability to design new materials from quantum-mechanical principles with computers is currently one of the fastest growing and most exciting areas of theoretical research in the nation and at LLNL. Our efforts are addressing problems in many disciplines, including physics, chemistry, materials science, and biotechnology.

Computer simulations are, of course, not new. Examples that have become familiar to the general public include simulating crash tests for the automotive industry, simulating aircraft in flight, and predicting the effects of earthquakes on large structures, such as bridges. (All three topics are described in the September–October 1993 issue of *Energy and Technology Review*.) In these cases and many others, computer simulations tell us not merely what might happen, but what actually will happen in the real world. This issue of *E&TR* highlights several in-house efforts involving atomic-scale computer simulations and features some of our ongoing collaborations with industrial partners. These efforts focus on simulations that explore problems at the fundamental, microscopic level.

The ultimate objective of a scientist involved in modeling and simulating materials at the microscopic level is to answer the following types of questions: What is matter really like at the atomic level? How can we modify the bonding between atoms to create novel materials with optimized properties? How can bulk materials be combined to exhibit new, desirable properties absent in the starting constituents? In addressing such questions, the scientist is armed with the set of laws that govern matter at the microscopic level, namely, quantum theory.

Matter is made of atoms, and atoms are made of nuclei surrounded by electrons. The basic laws governing the behavior of nuclei and electrons were formulated in the 1920s and are collectively known as quantum theory. Quantum theory forms the basis of our microscopic understanding of the physical universe. Equipped with the laws of quantum theory and a powerful computer, why not attack the formidable task of designing novel materials by doing calculations on every atom in the material until we arrive at the properties we need?

Unfortunately, such a straightforward approach is impossible. It is true that the quantum mechanical equations governing the behavior of electrons can be written in a relatively compact form. However, practical calculations become exceedingly difficult because of the large number of degrees of freedom and interactions between particles. Even the smallest speck of matter visible to the unaided eye contains several billions of electrons, and the complexity of their motion is enormous. Because electrons are charged and repel one another, the motion of each electron depends on the motion of all the others. To make the problem even more difficult, the laws of quantum theory tell us that each electron is described by a wave function. As a result, electrons behave like a pattern of crisscrossing waves on a rough sea. An exact calculation of a system with such mind-boggling complexity is far beyond the capacity of the most powerful computers.

Instead of attempting an exact—and ultimately impossible—calculation, scientists approximate physical laws to yield a feasible, yet somewhat inexact, calculation. The key to the spectacular success of modern quantum

simulations of materials is that the degree of inexactitude is quite small and can be controlled.

A breakthrough in the field occurred in the early 1960s with the formulation of density functional theory. The basic postulate of this important theory is that the ground-state energy (i.e., the lowest energy state) of a system of electrons moving in a given external potential can be obtained from a knowledge of the electron charge density. This concept offers tremendous computational advantages because the electron density becomes the basic variable rather than the complicated many-body wave function of all the electrons. Moreover, this powerful theory reduces the problem of describing the tangled, mutually dependent motion of electrons to one of describing the motion of a single, independent electron in an effective potential. In other words, we can describe the complex effects of all the other electrons on a single electron by an effective potential in which that electron moves. This simplified, but rigorous, description means that we can treat electrons as if they are independent of each other without seriously upsetting the result. The framework of the density functional theory gives us an extremely powerful and accurate technique to calculate the properties of materials on a first-principles, or *ab initio*, basis—that is, from the identities of the atoms making up a material and the laws of quantum theory.

Density functional theory, coupled with rapidly increasing computing power, led to an explosion of activity in the calculation of the properties of materials using the laws of quantum theory. By the early 1980s, it had become clear to the scientific community that the properties of simple crystals could be calculated with amazing accuracy using nothing but these laws. Soon, researchers began reproducing many material properties that previously could only be determined through experiments. Examples include the spectrum of atomic vibrations in solids, changes in crystal structure induced by applying external pressure, and the optical, electronic, and magnetic properties of materials. Researchers around the world reported similar successes for a wide variety of materials. What we learned is that computer calculations based on the microscopic laws of quantum theory really could tell how actual materials behaved.

But there is a catch or two to this approach. Even with the tremendous advances that emerged from density functional theory, large-scale dynamic simulations of materials and processes on a truly first-principles basis remains a formidable task. Moreover, it is not possible to apply first-principles methods to systems at nonzero temperature, where the electronic properties must be averaged over the many possible configurations of ions making up a system.

Fortunately, our first-principles knowledge of how electrons and nuclei interact in materials can be used as the basis to derive simple, yet accurate, models to reproduce the interactions. Once the model interaction potentials between atoms in materials are derived, it is possible to perform molecular dynamics simulations of complex materials processes based on the numerical calculation of atomic trajectories. Molecular dynamics simulations are usually based on empirical potentials that mimic the interatomic potentials in real materials. The simplicity that follows from using parameterized potentials is then exploited to treat large numbers of atoms (up to hundreds of millions) in more complex configurations. By controlling temperature (the mean velocity at which the constituent atoms move) during a molecular dynamics simulation, technologically interesting processes can be studied. These processes include melting, crystal growth and epitaxy, ion implantation, laser annealing, and defect motion. Thus, molecular dynamics simulations bridge the gap between quantum theory and statistical physics.

Accompanying the rapid pace of theoretical developments is another trend that is at the origin of the vitality of the field of materials physics today. In recent years, we have seen extraordinary advances in the ways materials can be synthesized. Advanced synthesis tools now allow us to fabricate materials atom by atom so that we can grow thin films, build multilayers, and construct many other products, such as fullerenes (in which the building block is C_{60}). Indeed, it is the intimate synergy between our ability to predict accurately from quantum theory how atoms *can* be assembled to form new materials and our capacity to *actually* synthesize novel materials atom-by-atom that gives the field its extraordinary intellectual vitality.

At LLNL, we are working on both sides of the equation by pursuing the theory of large-scale modeling as well as powerful methods to construct new materials with optimized properties. Many of our materials theory, modeling, and simulation activities are being done in collaboration with industrial participants in support of technology transfer initiatives.

Until now, materials design and processing have been, for the most part, empirical sciences. What this really means is that the process of coming up with an optimal material has been quite slow. For example, about one cancer drug in 40,000 has clinical significance, and perhaps one in a million would be curative. Using the old empirical methods, we can screen about ten thousand drugs a year.

At that rate, it could take 100 years to obtain our first cancer-curing drug. Designing materials by computer will accelerate this process by improving our understanding of the mechanisms by which carcinogenic molecules cause cancer. Computers will also enable the design of drug molecules that either inhibit these mechanisms or remove the carcinogenic molecules from our body.

Consequently, in designing new materials through computer simulations, our primary objective is to rapidly screen possible designs to find those few that will enhance the competitiveness of U.S. industry or have other positive benefits to society. Examples include screening of cancer drugs, advances in catalysis for energy production, design of new alloys and multilayers, and processing of semiconductors. The expertise resident at LLNL in the applied sciences, computations, and materials modeling puts us in a unique position to address these classes of problems.

At present, we face many challenges. Engineering new electronic materials is both costly and time-consuming today. We are still unable to design new alloys and polymers to meet application-specific requirements. Being able to do so quickly and at low cost would give the U.S. a tremendous edge in the international marketplace by providing American industry with revolutionary new capabilities. The national laboratories, with their world-leading competencies in advanced materials modeling, will play a central role in this process.

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